Stretch Efficiency for Combustion Engines: Exploiting New High-Dilution Combustion Regimes

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Galen B. Fisher (subcontractor)

University of Michigan

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DOE Management Team
Gurpreet Singh and Mike Weismiller

ORNL is managed by UT-Battelle, LLC
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Project Overview

Budget

- FY18: $300k
- FY19: $300k

Barriers

USDRIVE Roadmap, Topic Area 1: Dilute Gasoline Combustion

- Thermal management (efficient low-cost waste-heat recovery…)
- Increase EGR dilution tolerance
- Knock mitigation

Timeline

- Part of ORNL's FY17-FY19 lab call
- New lab call beginning FY19, proposing continuing work
- Builds on prior Stretch Efficiency research program at ORNL

Collaborators

- Precision Combustion, Inc. – Catalysts
- Umicore – Catalyst Coatings
- Ford – Providing technical input
- Caterpillar – Providing technical input
- FCA – Providing technical input
- AEC working group led by SNL
  - Industry feedback
- Aramco Services – Technical collaboration
- ANSYS (formerly Reaction design) – CFD model development

Universities

- University of Michigan - Galen Fisher
- Ghent University – Sebastian Verhelst

National Labs

- SNL - Isaac Ekoto

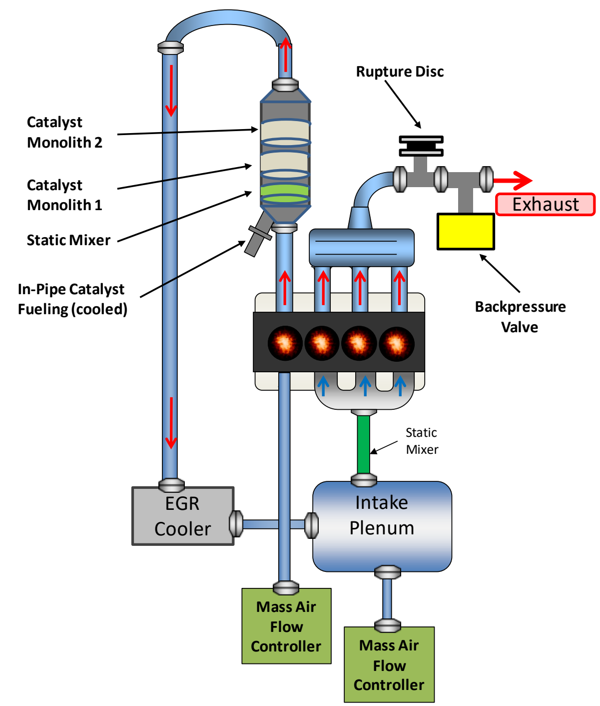
Relevance: Decreased Petroleum Consumption through Higher Engine Efficiency

Overall Project Goal

- Increase IC engine efficiency with an approach centered on thermodynamics of engine processes and minimizing losses
- Project focuses on efficiency gains under stoichiometric conditions to maintain compatibility with three-way catalyst

USDRIVE Roadmap, Area 1, Research Priorities Addressed

- Thermal management (efficient low-cost waste-heat recovery)
  – This project is investigating the feasibility of waste-heat recovery through thermochemical recuperation (TCR)
- Increase EGR dilution tolerance
  – EGR-loop catalytic reforming produces H_2 and CO, demonstrated EGR dilution tolerance of over 40% under stoichiometric A/F
- Knock mitigation
  – High EGR and reformed fuel alters knock kinetics



Note: Schematic represents engine flow paths and is not intended to represent instrumentation or controls

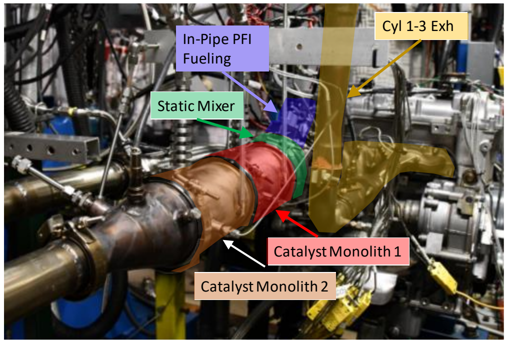
Resources

Budget

- **FY18: $300k**
- **FY19: $300k**

ORNL Personnel

- **PI: Jim Szybist, ORNL**
- **Synthetic Exhaust Flow Reactor Lead: Josh Pihl**
- **ORNL Contributors: Shean Huff, Brian Kaul, Melanie Debusk**



Subcontracts

Galen Fisher, University of Michigan

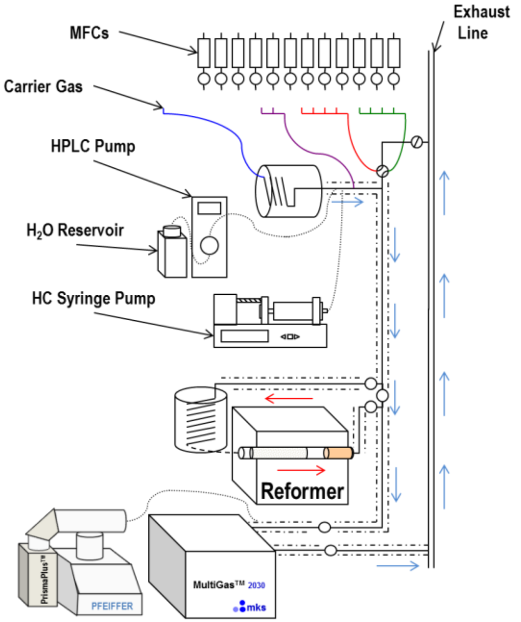
- **Consulting on catalyst materials and catalyst results**

Precision Combustion, Inc.

- **Supplying catalyst materials**

Equipment

- **Engine dynamometer laboratory**
  - **Multi-cylinder DI turbo engine**
  - **Custom intake and exhaust systems**
  - **5-gas emissions bench, FTIR, mass spectrometer**
- **Synthetic exhaust flow reactor laboratory**
  - **Well controlled synthetic exhaust composition using MFCs**
  - **Well controlled catalyst thermal boundary conditions**
  - **FID, FTIR, mass spectrometer**



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This Project has One Tracked Milestone for FY19

Fourth Quarter, FY2019

Complete evaluation of TCR potential at four different space velocity/inlet temperature conditions, representing four different engine speed-load conditions using the synthetic exhaust bench-flow reactor installation.

Status: On-track.

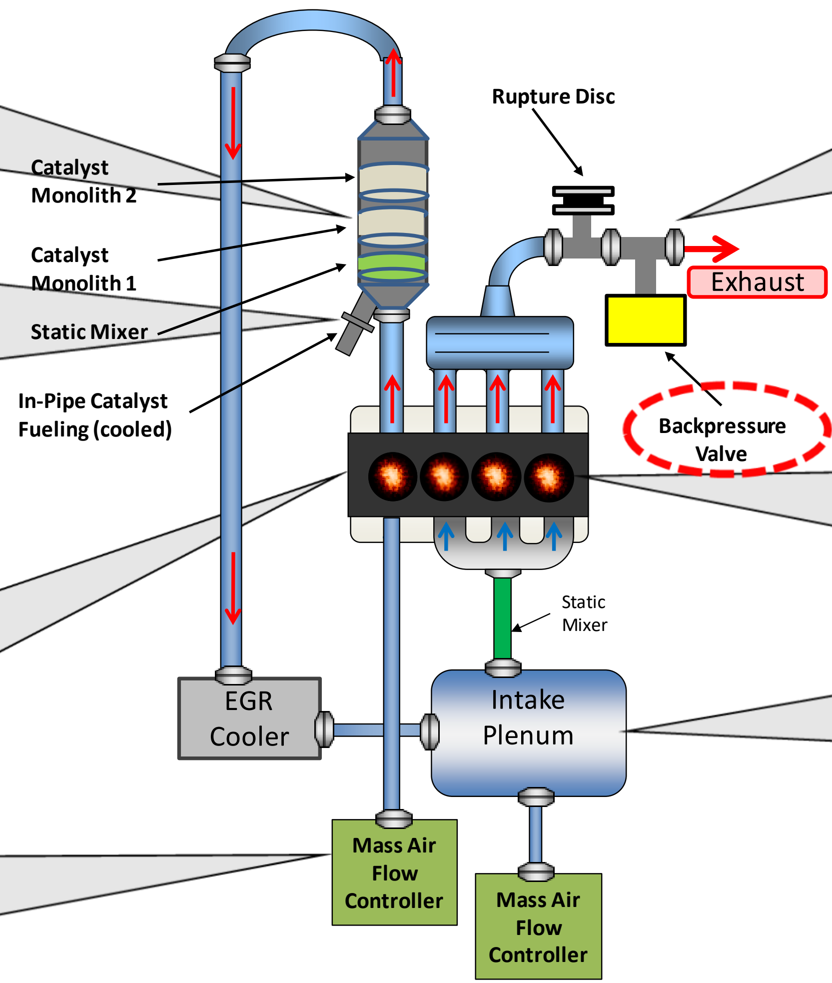
Approach: Engine Experiments, Guided by Thermodynamic Analysis by Flow Reactor Studies, Measure BTE

- Fuel reforming catalyst and EGR cooler
- Instrumented for temperature
- Species sampling

- Entirety of fuel-lean exhaust to feed reforming catalyst
- In-pipe fuel addition for fueling
- Fuel rich at catalyst entrance

- Load-balanced IMEP across all 4 cylinders
- Studies performed with full boiling range E10 gasoline

- Fresh air metered to cylinder 4
- Cylinder 4 operated fuel-lean
- **No EGR** in cylinder 4



- Stoichiometric exhaust
- Backpressure valve to simulate desired turbocharger efficiency

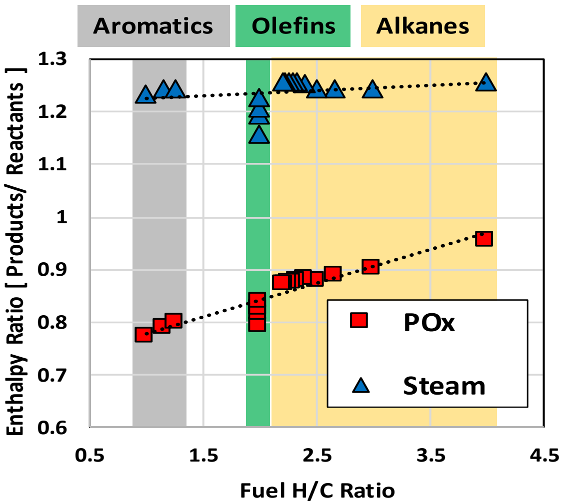
- Cylinders 1-3 operate high EGR dilution with reformate
- Stoichiometric air-fuel ratio

Intake plenum for cylinders 1-3 mixes fresh air with entirety of cylinder 4 exhaust and reformate

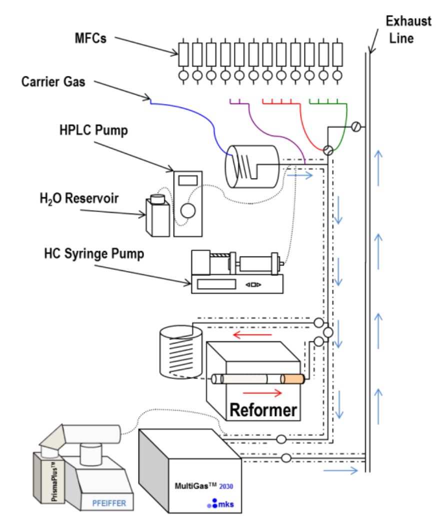
*Additional information in backup slides

Approach: Thermodynamics and Synthetic Exhaust Flow Reactor Provide Fundamentals and Path Forward

- Thermodynamic analysis of reforming processes on energy balance and engine cycles
  - 1st and 2nd Law energy balances with different reforming processes (partial oxidation (POx), steam, dry, non-equilibrium)
  - Relationship between molar expansion ratio (MER) and enthalpy-to-exergy ratio
  - Impact of reformate on thermodynamic cycle analysis, including specific heat ratio changes during compression and expansion

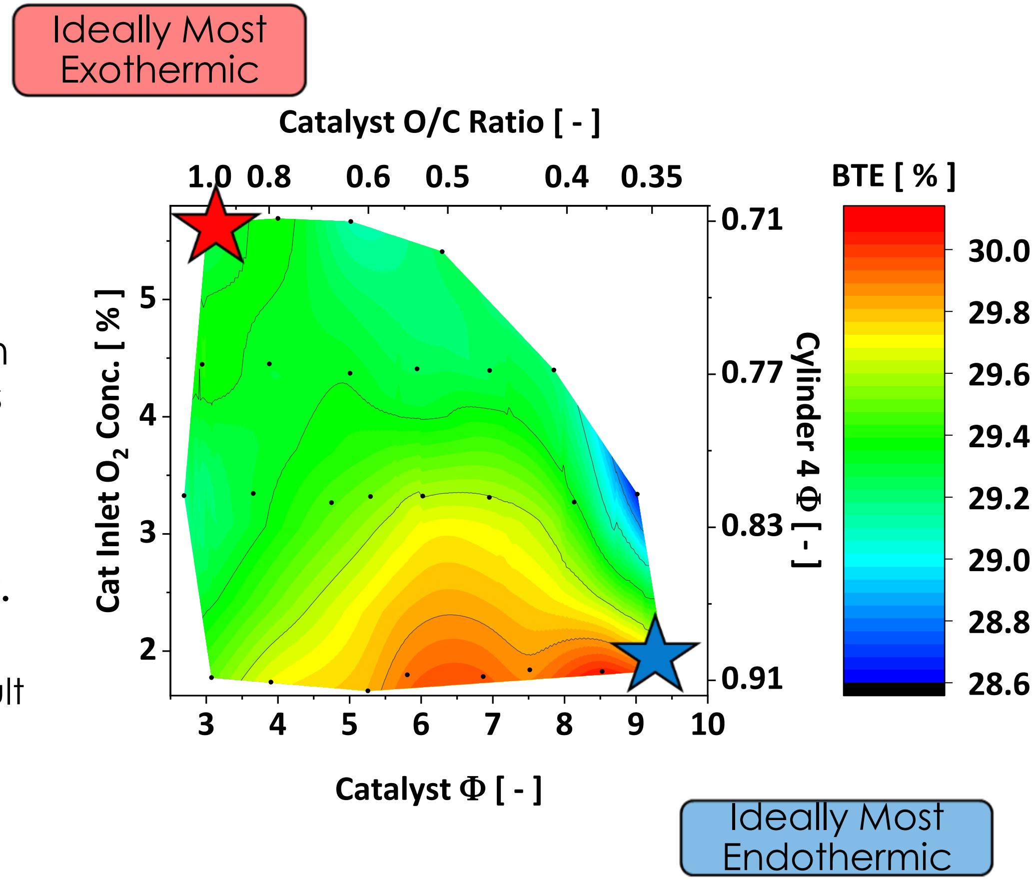


- Steam and partial oxidation reforming investigated in an automated synthetic exhaust flow reactor for application in an EGR-loop reforming strategy on a SI engine
  - Identifies catalyst boundary conditions for efficient reforming, including thermochemical recuperation
  - Engine operated to mimic the catalyst boundary conditions
  - Excellent transferability has been demonstrated



Moderate Speed and Load Condition Used to Baseline Catalyst Thermal State Prior to Increasing Loads

- Reforming increases efficiency above baseline (28.5% BTE) for all points
- Results show peak efficiency at low catalyst inlet O_2 and high catalyst equivalence ratio ($\Phi > 6$)
- Low inlet O_2 minimizes partial oxidation (exothermic) reforming and maximizes steam reforming (endothermic)
  - Exothermic reactions consume fuel energy in catalyst where it isn't converted to work. **Bad for efficiency.**
  - Endothermic reactions that convert exhaust heat to chemical energy result in waste heat recovery (thermochemical recuperation). **Good for efficiency.**
- **Robust reformer performance requires some O_2 and POx**

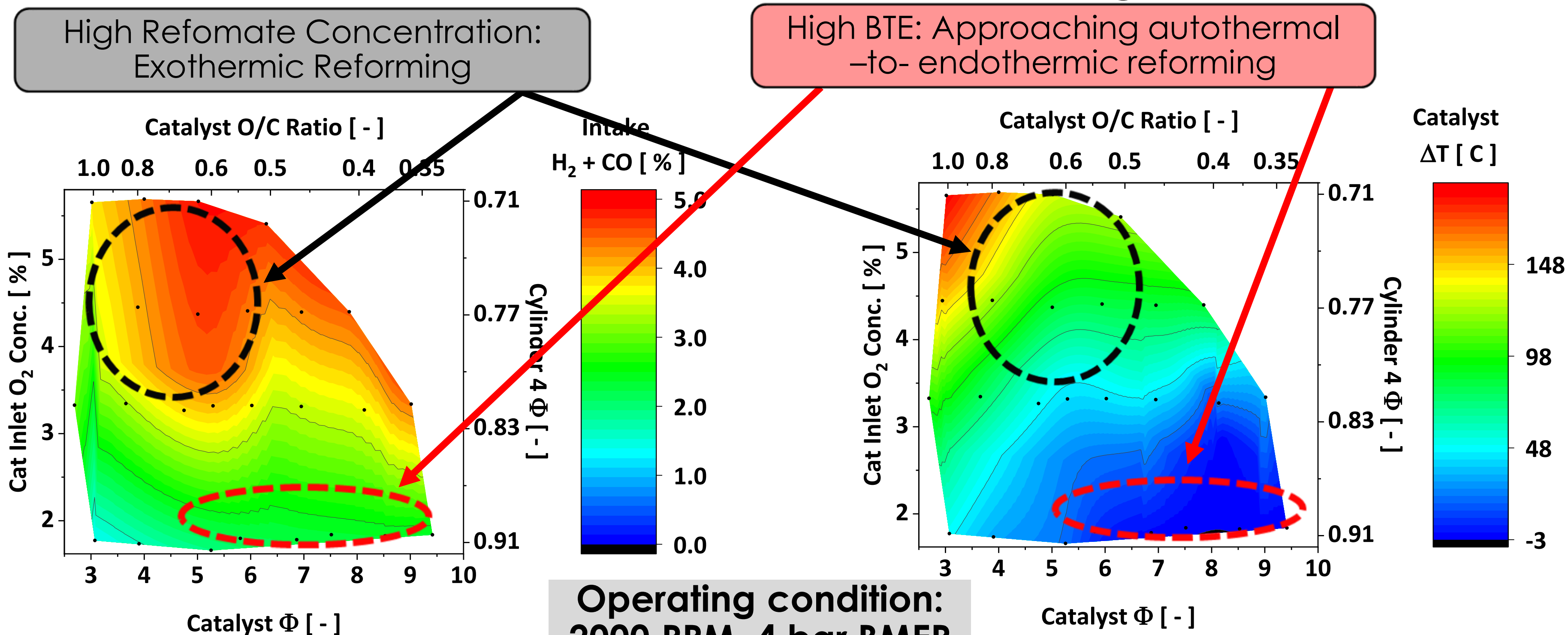


Operating condition: 2000 RPM, 4 bar BMEP

Accomplishments (1/10)

*Conditions in contour plots are at the reforming catalyst inlet

Peak Reformate Concentrations Do Not Result in Highest Efficiency Because of Inefficient Reforming



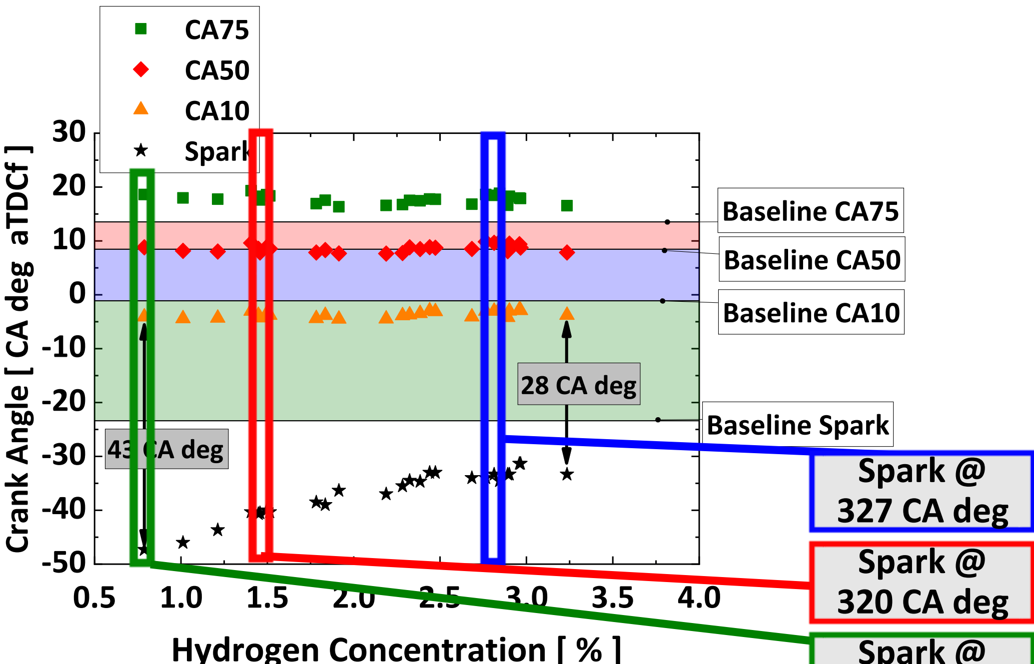
Operating condition: 2000 RPM, 4 bar BMEP

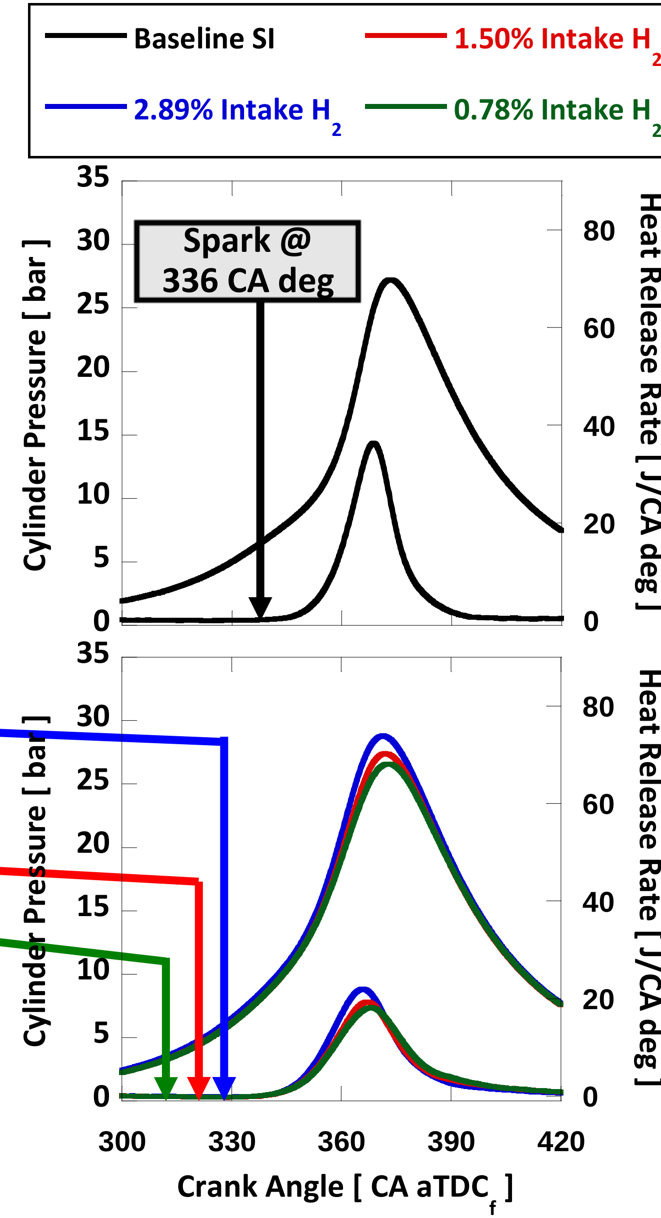
- Inlet O_2 varied between 13.2 and 14.8 vol%, equivalent to up to 36% EGR (backup slide)
- Stable combustion throughout operating range, <3% COV of IMEP (backup slide)
- Peak reformate concentrations occur in regions with high inlet O_2 concentration
  - High reformate conc. reliant on exothermic POx reforming, results in fuel consumption penalty
- Highest brake engine efficiency occurs with more modest H_2 (1.5-2.0 vol%) and CO (0.8-1.4 vol%) concentrations in the intake manifold

Accomplishments (2/10)

*Conditions in contour plots are at the reforming catalyst inlet

For Dilute Cylinders, Hydrogen Primarily Affects the Initial Flame Kernel Development





- Baseline condition has the shortest duration in all phases of the combustion process
- Spark timing advances as % H_2 decreases, but minimal impact on the remainder of the combustion event

Operating condition: 2000 RPM, 4 bar BMEP, various catalyst Φ and inlet O_2 concentrations

Accomplishments (3/10)

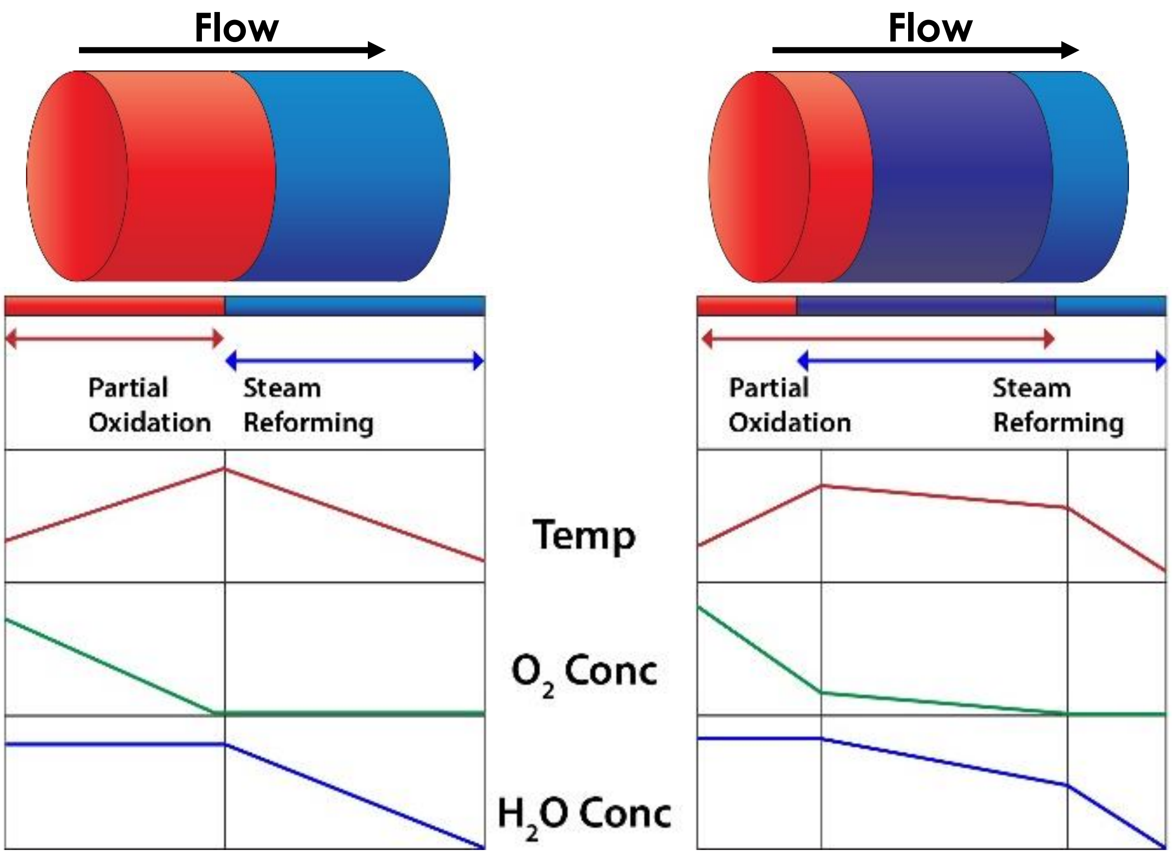
Does Oxidation Preferentially Occur Prior to Steam Reforming, or Are These Reactions Competitive?

Theory 1. Oxidation is Favored over Steam Reforming

- Exothermic reactions consume all oxygen prior to steam reforming
- In fuel-rich systems, exotherm is a function of oxygen concentration

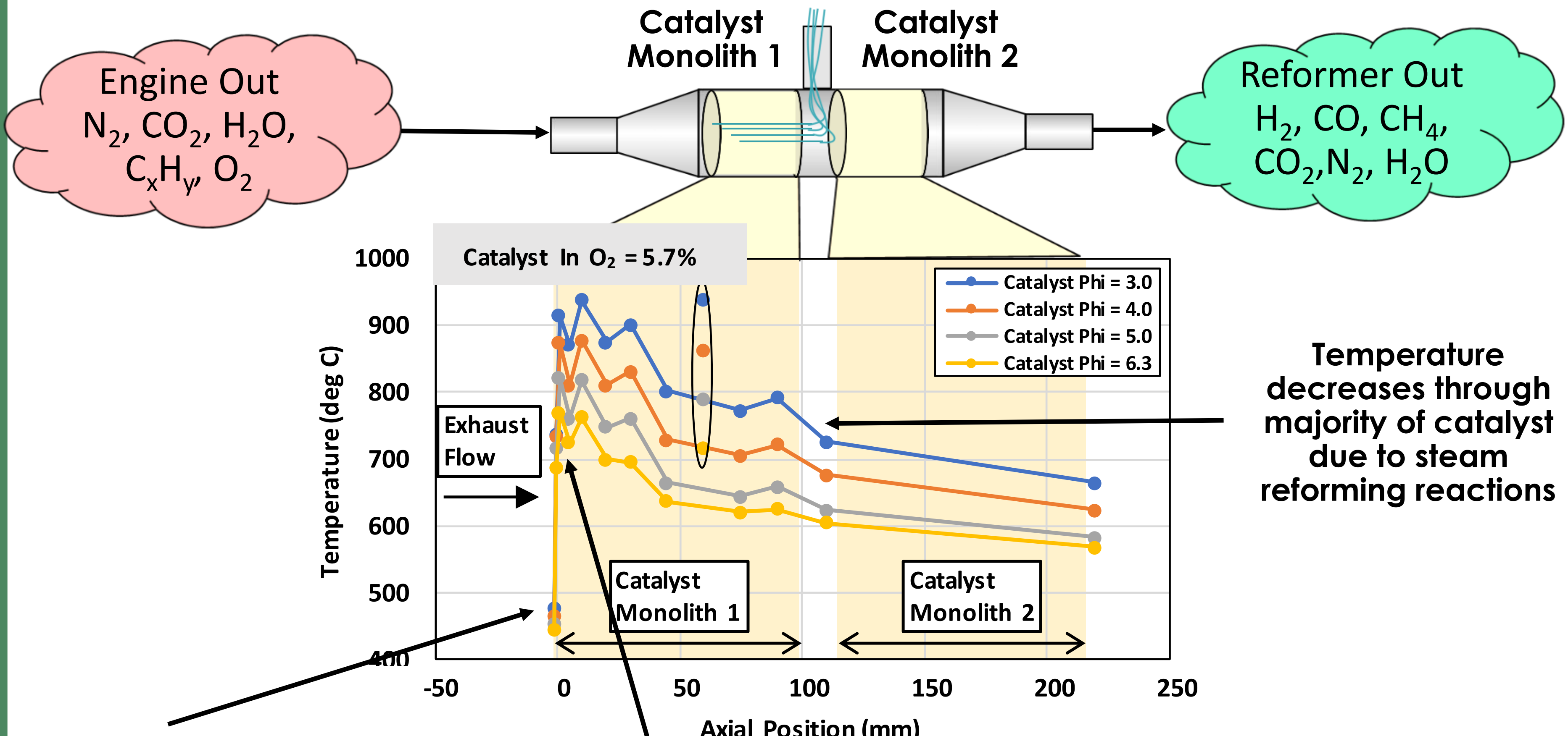
Theory 2. Oxidation and Steam Reforming are Competitive Reactions

- Endothermic steam reforming occurs at the same axial positions as exothermic partial oxidation reactions
- Competition for catalytic sites
- <u>Endothermic reactions moderate temperature, exotherm magnitude</u>



Accomplishments (4/10)

Reforming Catalyst Instrument for Axial Temperature Profile Provides Insights into Reforming Reactions



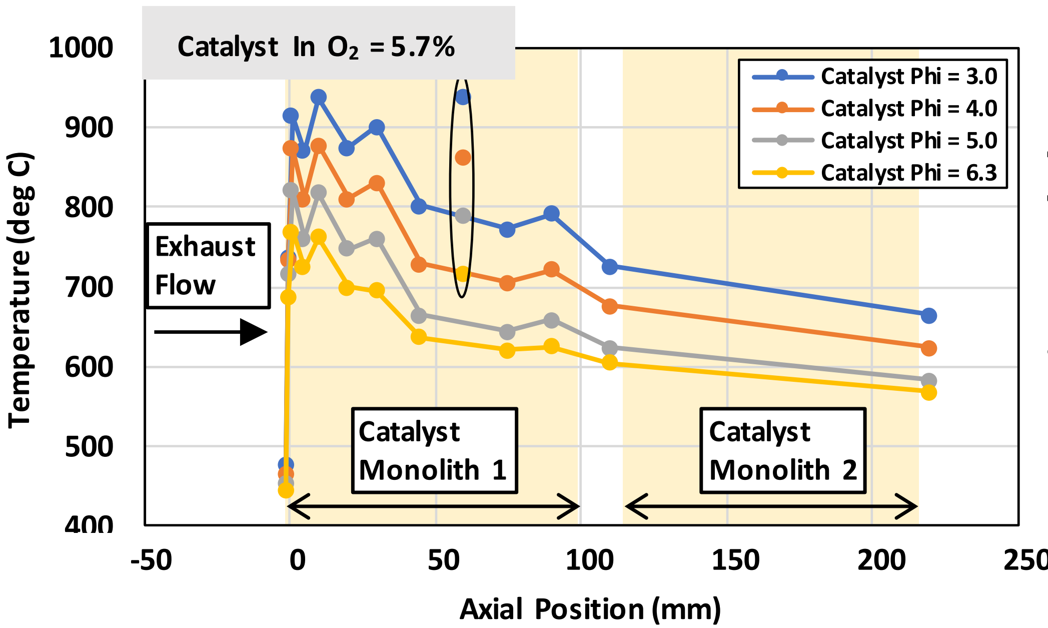
Temperature decreases through majority of catalyst due to steam reforming reactions

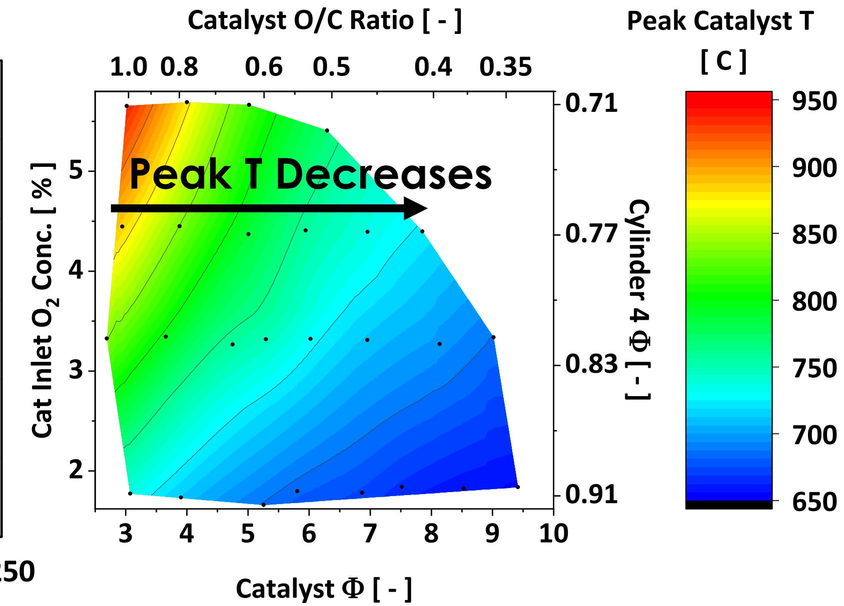
Engine Outlet T is Reformer Inlet T

Partial oxidation reactions cause temperature to increase at face of catalyst

Accomplishments (5/10)

At Constant Inlet O_2, Increasing Catalyst Φ Decreases Peak Catalyst Temperature





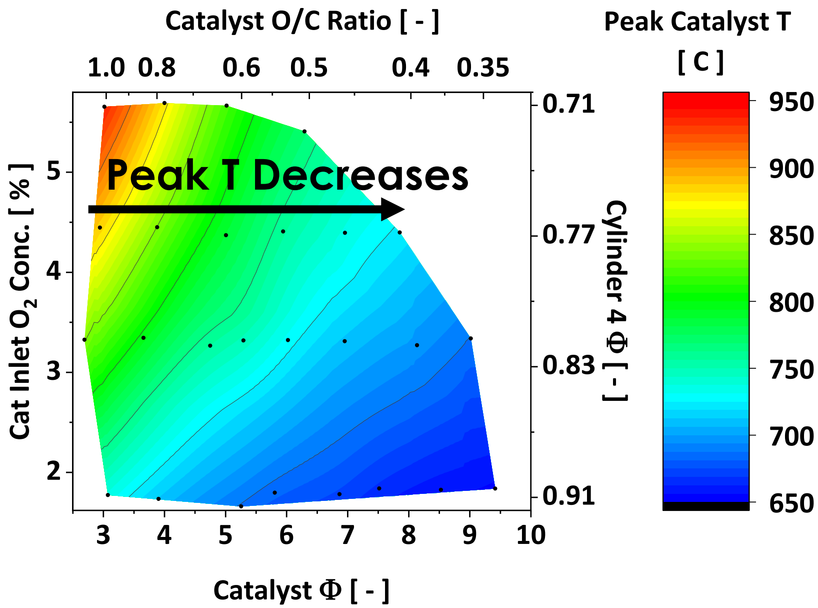
- All conditions experienced a large temperature increase at the front face of the catalyst (as high as 400 deg C within first several mm!)
- Temperature decreases with axial position due to endothermic reactions
- **Increasing Φ with constant catalyst in O_2 % results in a decrease of the peak catalyst temperature**

**Operating condition:
2000 RPM, 4 bar BMEP**

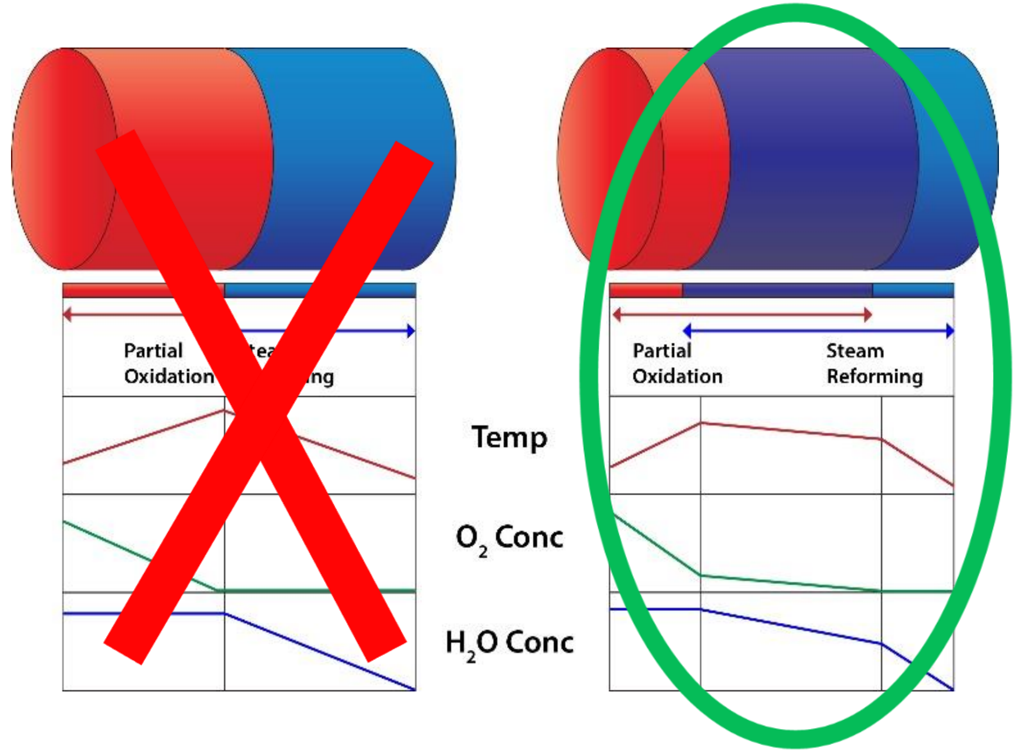
Accomplishments (6/10)

***Conditions in contour plots are at the reforming catalyst inlet**

Decreasing Peak Catalyst Temperature at Constant Inlet O_2 is Evidence that Steam Reforming is Competitive with Partial Oxidation



Operating condition:
2000 RPM, 4 bar BMEP

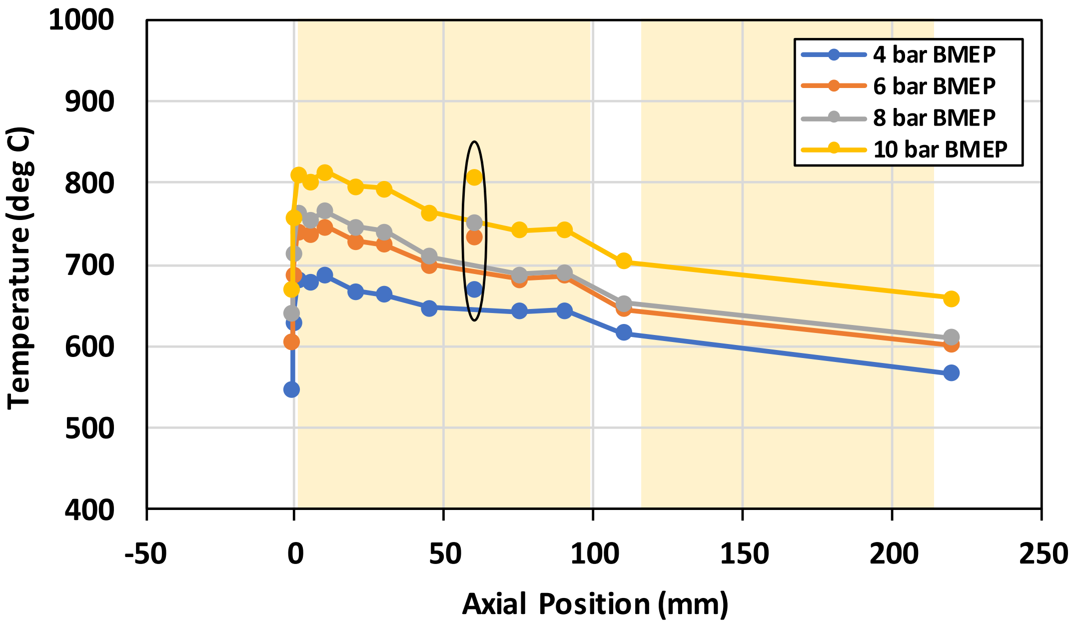


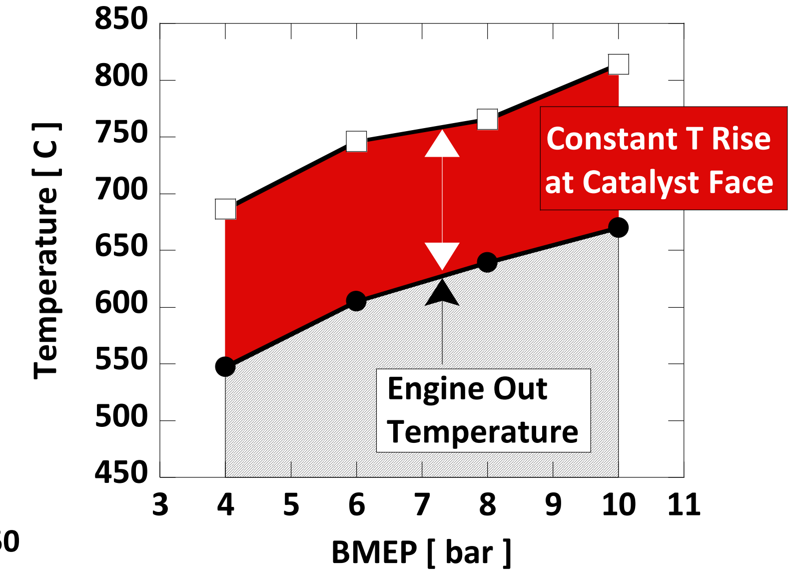
- O_2 conc. at catalyst inlet alone does not control peak catalyst temperature or ΔT
- Maximum catalyst temperature can be moderated by controlling a combination of catalyst Φ and inlet O_2, evidence of high activation energy for steam reforming rxns
- **Finding provides confidence to move to higher load operation without melting catalyst**

Accomplishments (7/10)

***Conditions in contour plots are at the reforming catalyst inlet**

Load Increases Confirm that Temperature Rise in Front Portion of Catalyst can be Controlled as Load Increases



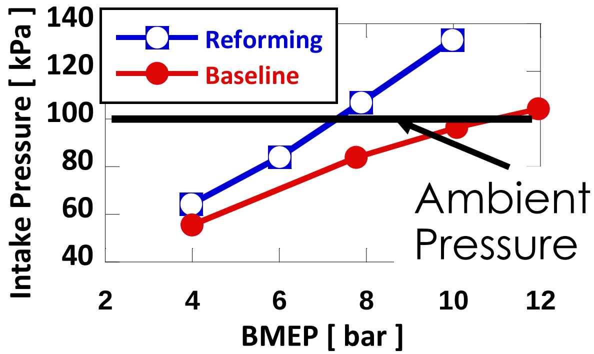


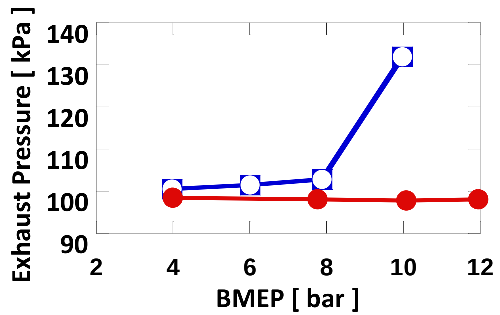
- Catalyst inlet temperature increases with load as expected
  - Catalyst inlet temperature is the exhaust temperature from cylinder 4
- Temperature increase at catalyst face remains constant as load increases
  - Catalyst substrate is rated for ~1200 deg C

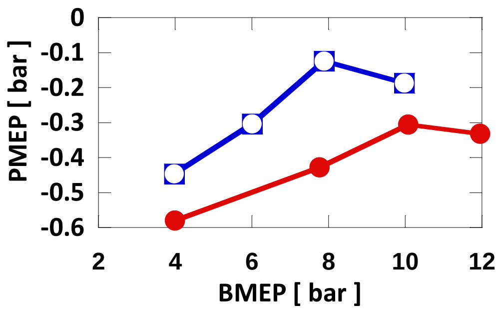
Operating condition:
Load Increasing from 4 to 10 bar BMEP with catalyst O_2 = 1.8% and Catalyst Φ = 5.0

Accomplishments (8/10)

As Load was Increased, Realistic Air Handling Boundary Conditions were Maintained (Turbo Efficiency = 40%)







- High dilution combustion process required boosted at lighter engine load than baseline operation (7.5 bar BMEP vs. 11 bar BMEP)
- With boosted operation, simulated a combined turbo efficiency of 40%
  - Increased backpressure based on boost pressure and exhaust T to achieve desired turbo efficiency
- Pumping work advantage for reforming condition exists, but diminished with boost

Operating condition:
Load Increasing from 4 to 10 bar BMEP with catalyst O_2 = 1.8% and Catalyst Φ = 5.0

Accomplishments (9/10)

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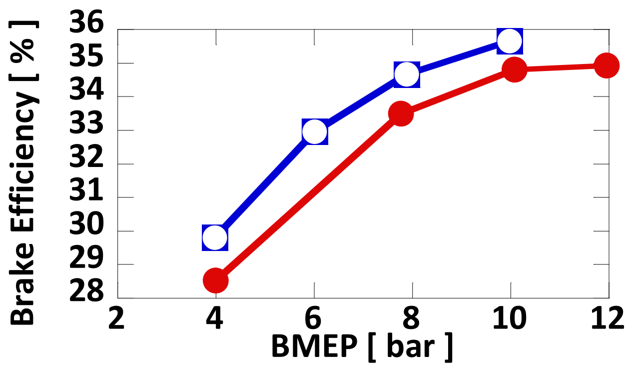
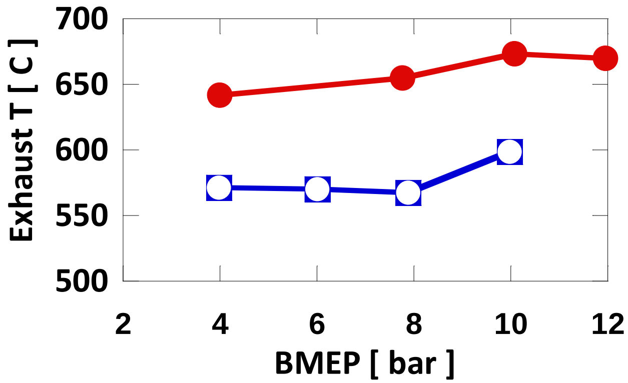
Brake Efficiency Benefit Realized Over Full Engine Load Range Investigated

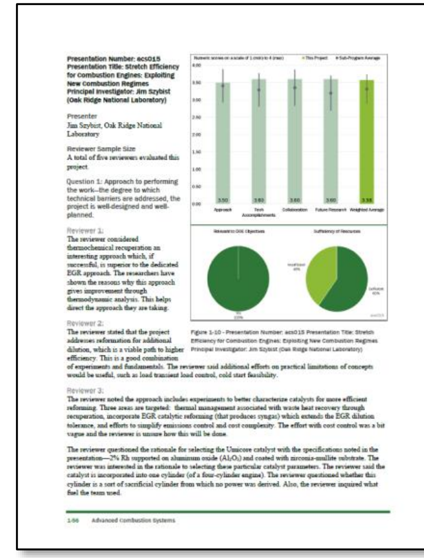
- Brake efficiency increase of 1-2 efficiency points at conditions investigated
- Previous investigations showed similar benefits at additional operating conditions
  - Near-idle (1500 rpm, 0.7 bar BMEP)
  - Higher speed (2500 rpm, 6 bar BMEP)
- Higher efficiency results in exhaust temperatures nearly 100 deg C lower than baseline condition
  - Exhaust T sufficiently high for 3-way catalyst operation
- Benefits achieved with stoichiometric exhaust conditions, compatibility with and 3-way catalysts
  - Conventional stoichiometric cold-start for 3-way catalyst light-off
- Room for optimization for additional benefits
  - Knock benefit through high EGR and reformate, allow for higher compression ratio
  - Higher turbulence geometry for reduced combustion duration





Accomplishments (10/10)

Five Reviewers Evaluated this Project in 2018
Overall Positive Comments with Room for Improvement


Presentation Number: acs015
Presentation Title: Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes
Principal Investigator: Jim Szybist (Oak Ridge National Laboratory)

Presenter
Jim Szybist, Oak Ridge National Laboratory

Reviewer Sample Size
A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer considered thermochemical recuperation an interesting approach which, if successful, is superior to the dedicated EGR approach. The researchers have shown the reasons why this approach gives improvement through thermodynamic analysis. This helps direct the approach they are taking.

Reviewer 2:
The reviewer stated that the project addresses reformation for additional dilution, which is a viable path to higher efficiency. This is a good combination of experiments and fundamentals. The reviewer said additional efforts on practical limitations of concepts would be useful, such as load transient load control, cold start feasibility.

Figure 1-10 - Presentation Number: acs015 Presentation Title: Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes Principal Investigator: Jim Szybist (Oak Ridge National Laboratory)

Reviewer 3:
The reviewer noted the approach includes experiments to better characterize catalysts for more efficient reforming. Three areas are targeted: thermal management associated with waste heat recovery through recuperation, incorporate EGR catalytic reforming (that produces syngas) which extends the EGR dilution tolerance, and efforts to simplify emissions control and cost complexity. The effort with cost control was a bit vague and the reviewer is unsure how this will be done.

The reviewer questioned the rationale for selecting the Umicore catalyst with the specifications noted in the presentation—2% Rh supported on aluminum oxide (Al_2O_3) and coated with zirconia-mullite substrate. The reviewer was interested in the rationale to selecting these particular catalyst parameters. The reviewer said the catalyst is incorporated into one cylinder (of a four-cylinder engine). The reviewer questioned whether this cylinder is a sort of sacrificial cylinder from which no power was derived. Also, the reviewer inquired what fuel the team used.

1-56 Advanced Combustion Systems

A reviewer questioned whether the cylinder that fed the catalyst was a sacrificial cylinder with regards to power production.

All of the cylinders produced the same amount of power, with balanced IMEP across all four cylinders. This cylinder only differs from the other cylinders in terms of composition and combustion duration.

A reviewer questioned hardware modifications were required for higher loads

Higher engine loads required boosting the engine. It was previously setup as a naturally aspirated engine. Further, since the cylinder feed coming from three cylinders would be unbalanced for a turbocharger, it was necessary to simulate boost. This required air flow control, additional backpressure, a higher capacity EGR cooler.

A reviewer questioned the rationale for selecting the Umicore catalyst.

The selection was based on literature showing that Rh-based reforming catalysts are the most sulfur-tolerant in addition to input from our catalyst consultant, Galen Fisher. We are adding a Rh-based catalyst on a metal substrate (PCI catalyst) in 2019.

The reviewer commented that it would be useful to present more than cause-and-effect results and try to explain what is happening.

Explanations of what is occurring is the goal of this project. In 2018, an analysis was done to examine why reforming alters the ratio of specific heat of the working fluid and the resultant impact on cycle efficiency. In this presentation, we have demonstrated that steam reforming reactions are competitive with partial oxidation reactions.

The reviewer questioned why the catalyst temperature increases with engine speed.

The effect of engine speed on exhaust temperature, and thus catalyst temperature, is that there is less time for heat loss to the coolant. This concentrates heat in the exhaust.

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Collaborations

- Precision Combustion Inc. (PCI) – Providing metal-substrate reforming catalyst
- Umicore – Providing pre-production Rh-based catalysts
- University of Ghent – Sebastian Verhelst providing modeling support on understanding the impact of molar expansion ratio
- AEC Working Group bi-annual meetings
  - Mechanism for industry feedback
- OEM Collaborations: one-on-one discussions, discussions of implementation barriers, feedback on results and future plans
  - Ford
  - Caterpillar
  - FCA
- University of Michigan: Galen Fisher advising on catalyst formulation and operating conditions through subcontract
- Related funds-in project with Aramco Services Co.
- Sandia National Laboratories: Historical collaboration with Isaac Ekoto (and Dick Steeper). Projects diverged this year, but technical discussions continue.
- Project direction from 2010 USCAR Colloquium

    http://feerc.ornl.gov/pdfs/Stretch_Report_ORNL-TM2010-265_final.pdf

Remaining Barriers and Future Work

Remaining Barrier 1

It is unclear if this technology can enable additional efficiency increases through knock mitigation at higher loads.

Corresponding Future Work

Substantial progress made in increasing the load since the 2018 AMR! We will continue to increase loads to maximize energy density (downsizing and downspeeding).

- **Catalyst from PCI will be used in 2019 (metal substrate) increased high-load compatibility (compact packaging, minimize differential thermal expansion)**
- **Higher compression ratio engine configuration (11.85 vs. 9.2)**

Remaining Barrier 2

Unclear how much fuel-borne sulfur will limit the applicability of this technology.

Corresponding Future Work

Characterize sulfur deactivation in controlled maner in flow reactor and engine studies

Remaining Barrier 3

Unclear the extent to which the lower molar expansion ratio of reformate limits potential efficiency benefits.

Corresponding Future Work

In collaboration with Ghent University, we will embark on an experimental engine campaign to investigate fuels with varying molar expansion ratios (0.85 to 1.08). Ghent University will support this work with thermodynamic modeling.

Any proposed future work is subject to change based on funding level

Summary

Relevance

Addressing multiple aspects of the USDRIVE Roadmap highest priority: Dilute Gasoline Combustion 1) low-cost waste heat recovery, 2) increased EGR tolerance, and 3) knock mitigation

Approach: Experimental and Modeling Efforts Grounded in Thermodynamics

Thermodynamic analysis of reforming and combustion processes, as well as synthetic exhaust flow reactor investigations guide engine experiment. The engine is operated so that the catalyst boundary conditions for efficient reforming are achieved.

Accomplishments: Substantial Progress in Increased Load Range while Maintaining Higher Efficiency

- *Demonstrated that endothermic steam reforming reactions are competitive with exothermic partial oxidation reforming reactions, thereby moderating the peak temperature in the catalyst*
- *Showed that the primary role of reformate was to reduce the early flame kernel development process, with little impact on latter stages of the combustion process*
- *The efficiency benefit of the EGR-loop reforming process could be maintained as engine load increases into boosted operation and while maintaining realistic turbocharger efficiency*

Collaborations

- *Catalyst interactions: Umicore for conventional catalysts, PCI for metal-substrate catalysts*
- *Industry interactions: AEC Program Review meeting, OEM one-on-one guidance*
- *University interactions: Starting new collaboration with Ghent University on Molar Expansion Ratio*

Future Work

- *Investigate knock mitigation benefits of EGR-loop reforming by pushing to higher loads and increasing the compression ratio*
- *Characterize sulfur deactivation*
- *Develop a better understanding of the thermodynamic impact of using a lower molar expansion ratio fuel (reformate) on engine efficiency*

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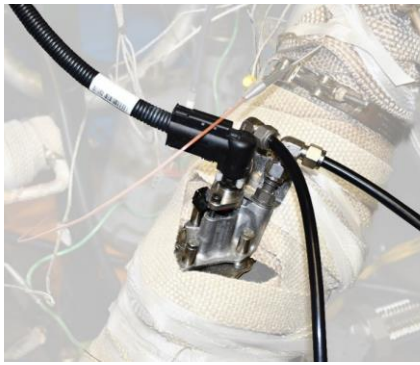
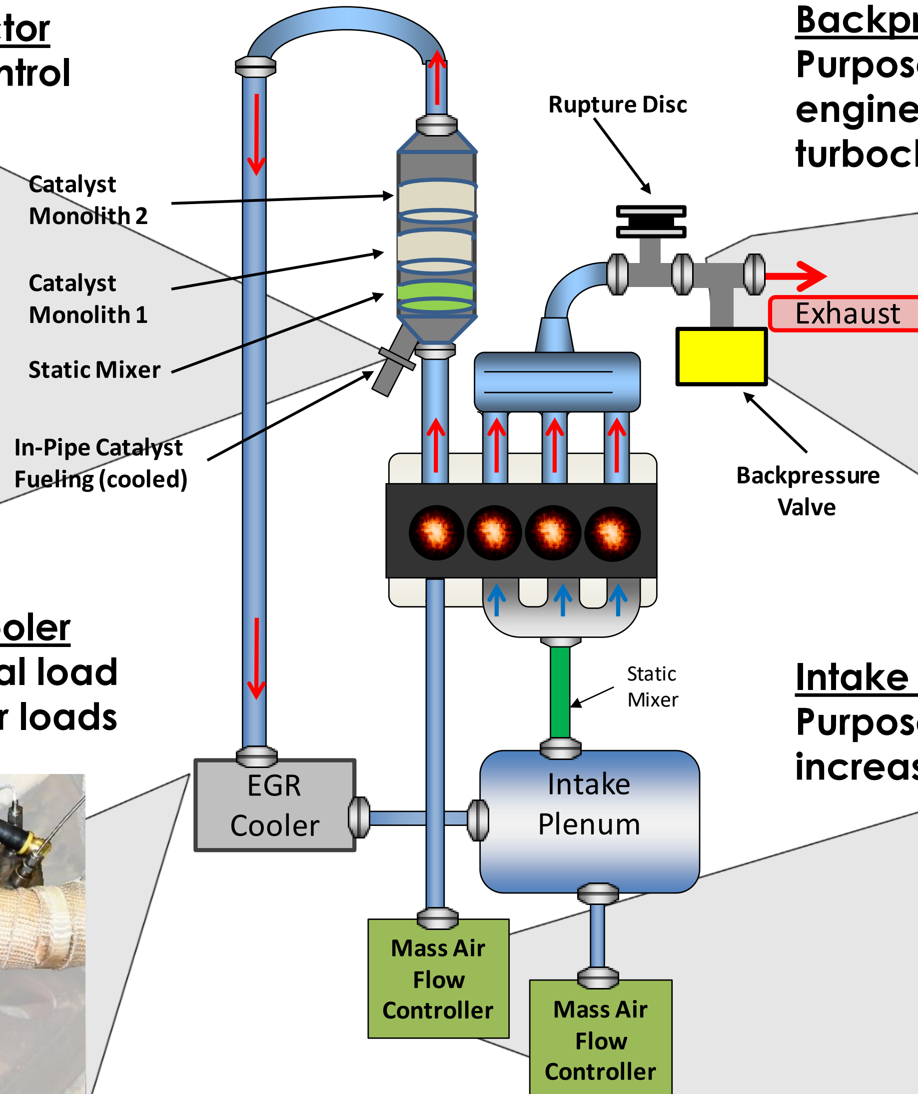
Technical Backup Slides

Backup Slide 1. Engine Modifications Required for Increasing Engine Load

Water-cooled PFI injector
Purpose: Improved control of $\Phi_{catalyst}$





Backpressure Valve
Purpose: Apply backpressure on engine under boost for realistic turbocharger boundary conditions

High Capacity EGR Cooler
Purpose: Higher thermal load in EGR loop with higher loads

Intake Air Mass Flow Controllers:
Purpose: Boost engine for increased load range operation

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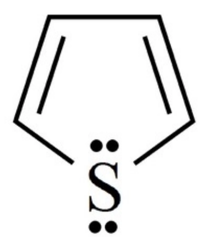
Backup Slide 2: Fuel Used was Representative with the Exception of Sulfur Content

- Euro EEE Stage IV Gasoline
  - Premium grade E10 gasoline
  - Realistic and representative concentrations of aromatics, olefins, paraffins, and ethanol
  - Realistic and representative distillation curve
  - Realistic and representative C/H/O
- Sulfur concentration isn't representative
  - 2 ppm sulfur is lower than realistic fuel
  - Marketplace currently in a transition from 30 to 10 ppm S for Tier III gasoline
- Using base fuel with very low sulfur allows this parameter to be isolated and investigated in several different ways
  - Several ml of thiophene mixed into a barrel of fuel increases S without changing base fuel formulation
  - Gaseous H_2S and SO_2 can be injected upstream of the catalyst directly

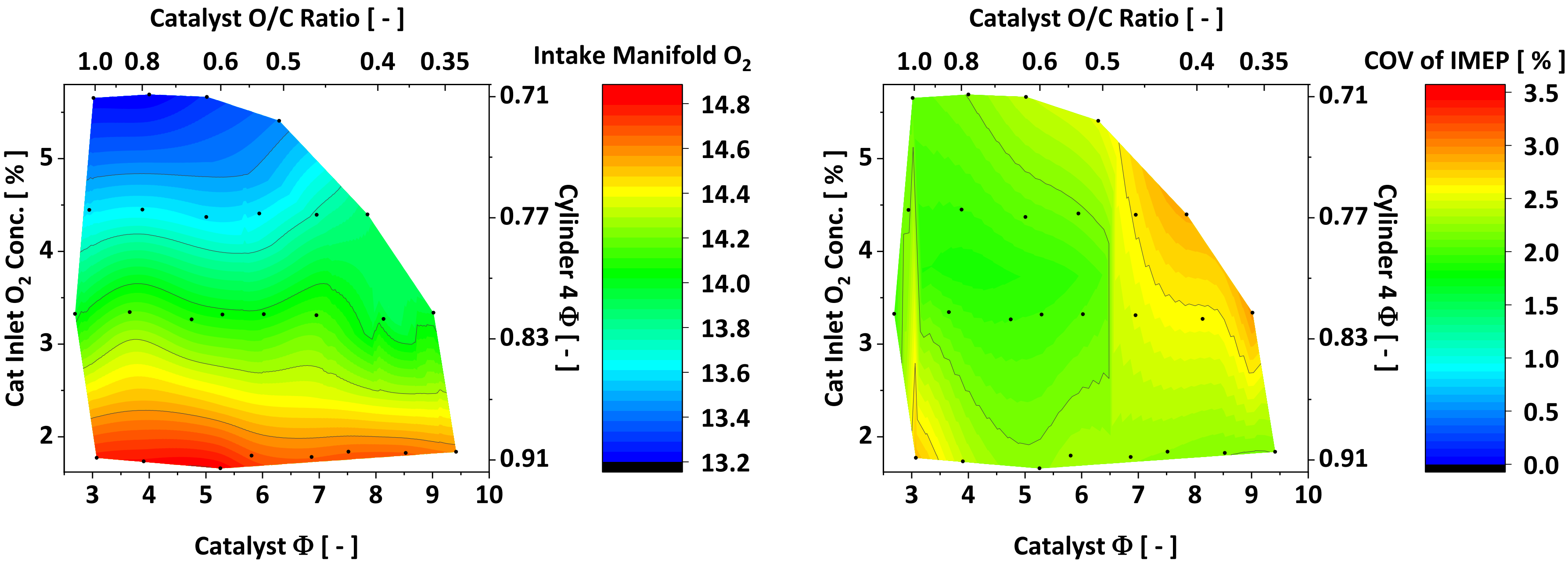
RON [-]	ASTM D2699	97.6
MON [-]	ASTM D2700	86.7
Anti-knock index (AKI) [-]	N/A	92.2
Ethanol [vol %]	ASTM D4815	9.5
Carbon [wt %]	ASTM D5291	83.03
Hydrogen [wt %]	ASTM D5291	13.49
Oxygen [wt %]	ASTM D4815	3.48
Net Heating Value [MJ/kg]	ASTM D240	41.5
Sulfur [mg/kg]	ASTM D5453	2
Aromatics [vol %]	ASTM D1319	28.4
Olefins [vol %]	ASTM D1319	8.2
Saturates [vol%]	ASTM D1319	53.9
Initial boiling point [°C]	ASTM D86	37
10% distillation [°C]	ASTM D86	54
50% distillation [°C]	ASTM D86	86
90% distillation [°C]	ASTM D86	155
Distillation end point [°C]	ASTM D86	174



Impact of sulfur on the reforming catalyst will be the subject of future investigations

Any proposed future work is subject to change based on funding level

Backup Slides 3: Reforming Combustion Strategy Capable of Maintaining Low Cyclic Variability with Very Low Intake O_2 (High EGR)



- Inlet O_2 varied between 13.2 and 14.8 vol%, equivalent to up to 36% EGR
- Despite high dilution levels, engine operation remains stable (<3% COV of IMEP)
- With conventional EGR, engine becomes unstable at 25% EGR or less

*Conditions in contour plots are at the reforming catalyst inlet

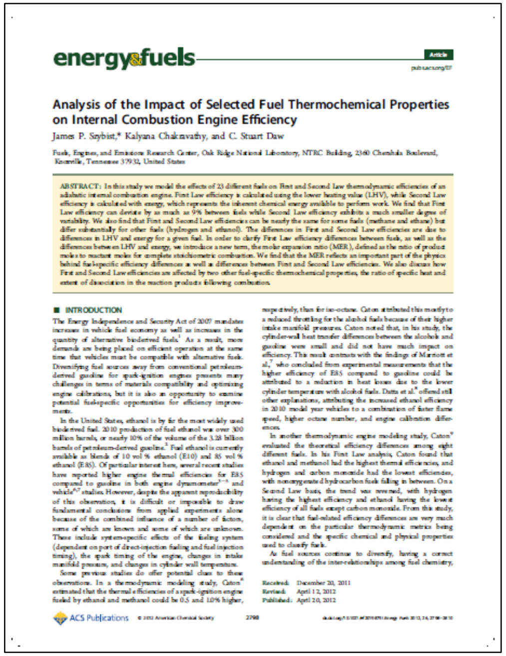
Backup Slide 4: Hypothesis: Exergy/enthalpy ratio is related to the molar expansion ratio

Molar Expansion Ratio ≡ (moles products)/(moles reactants)

- Molar expansion ratio is dependent on fuel type

$CH_4 + 2\ (O_2 + 3.76\ N_2) \longrightarrow CO_2 + 2\ H_2O + 7.52\ N_2$	$n_{product}/n_{reactant} = 1.00$
$CH_3OH + 1.5\ (O_2 + 3.76\ N_2) \longrightarrow CO_2 + 2\ H_2O + 5.64\ N_2$	$n_{product}/n_{reactant} = 1.21$
$CO + 0.5\ (O_2 + 3.76\ N_2) \longrightarrow CO_2 + 1.88\ N_2$	$n_{product}/n_{reactant} = 0.85$

  - The molar change during combustion is not accounted for in the LHV measurement or the enthalpy of reaction
  - Change in the number of moles is accounted for in the entropy term, so it is included in exergy of reaction
- Current study is limited to stoichiometric combustion with air to maximize fuel differences in molar expansion ratio
  - Molar expansion ratio approaches unity with increasing dilution (lower equivalence ratio or higher EGR)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Analysis of the Impact of Selected Fuel Thermochemical Properties on Internal Combustion Engine Efficiency

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Szybist, J.P., K. Chakravathy, C.S. Daw. *Analysis of the Impact of Selected Fuel Thermochemical Properties on Internal Combustion Engine Efficiency*. Energy & Fuels, 2012, vol 26(5), pp. 2798-2810.

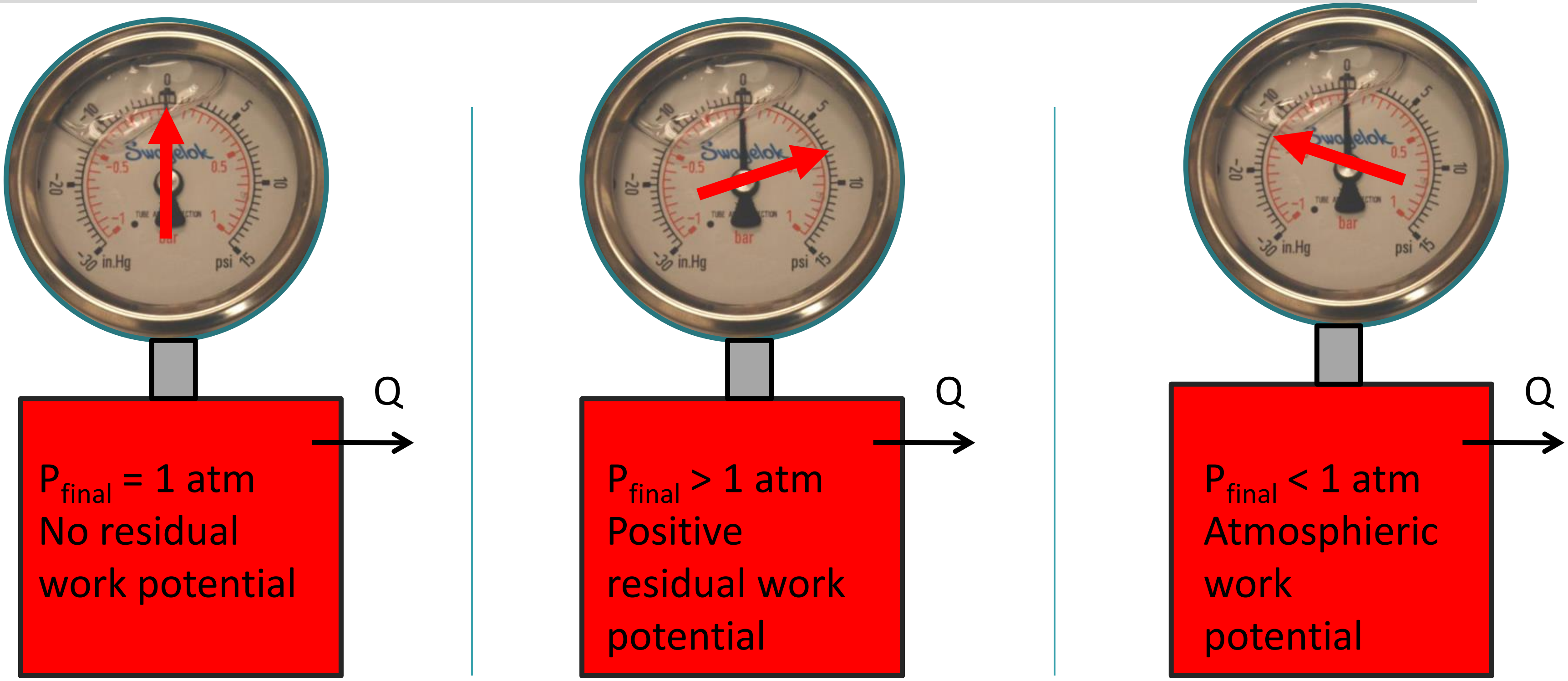
Molar expansion ratio determines the extent of residual pressure available to perform work

$CH_4 + 2(O_2 + 3.76\ N_2)$

$CH_3OH + 1.5(O_2 + 3.76\ N_2)$

$CO + 0.5(O_2 + 3.76\ N_2)$

Constant volume reactant chambers, Initial T = 100 C, Initial P = 1 atm



Final T = Initial T = 100 C